Robust, reproducible workflows for EC-Earth

Pablo Echevarria (pablo.echevarria@bsc.es)[1], Miguel Castrillo[1], and Mario Acosta[1]

[1]Computational Earth Sciences at the Earth Sciences department

Barcelona Supercomputing Center

The Earth Sciences department from the Barcelona Supercomputing Center (BSC) makes use of the EC-Earth model to run a wide range of experiments in different supercomputers as MareNostrum4, Nord3 and CCA. Switching platforms or combining different architectures in the same experiment is possible by using the **Autosubmit** workflow manager to control and automatize all the tasks needed to fulfill these simulations that are characterized by having **complex workflows**. All users in the community can take advantage of this approach to perform their simulations. The Auto-EC-Earth project is a set of templates and libraries that allows to automatize other tasks as the post processing (cmorization, ece3post-proc, etc) and archiving.

Simulations running at BSC

In the BSC we are committed to several projects, studying the climate at different scales, from seasonal to decadal, from coarse to very high resolution and studying different subsystems. All of these variety requires very different kind of experiments:

- OMIP, AMIP, GCM
- Earth system model
  - LPJG (land vegetation) HTESSEL (land surface)
  - NEMO (Ocean) PISCES (biogeochemistry)
  - TM5 (Atmospheric Chemistry)
- PISCES, ENKF (DA), Nudging (Ocean and Atmosphere)

Within some of these cases there are simulations using complex workflows combining different start dates and members for a number of steps or chunks. Some examples are or seasonal prediction experiments **running several start dates and members at the same time**:

- 1960 - 2018 start dates, 10 members , 11 years = **600 non independent simulations**.
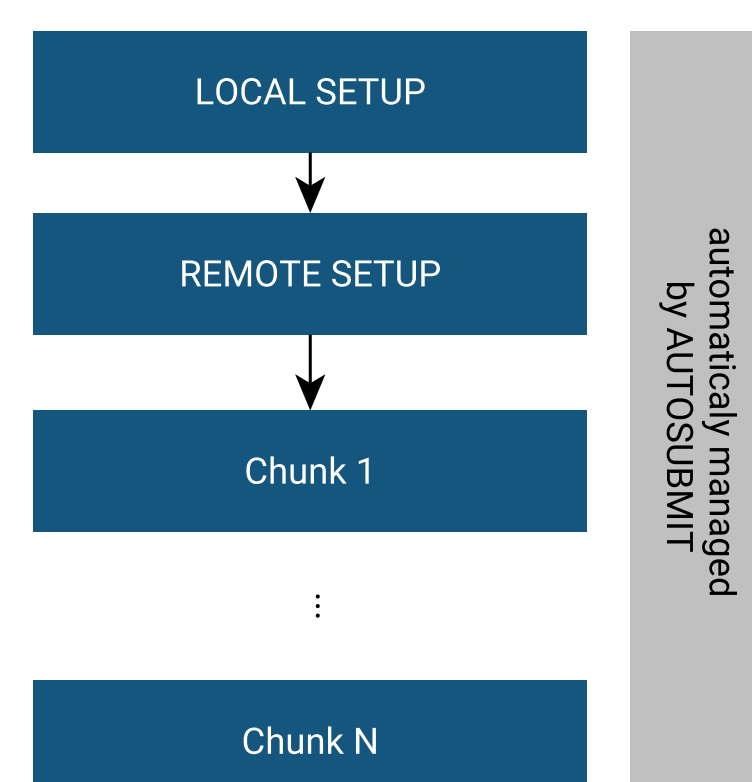
- 7 month simulations, 2 or 4 start dates per year (season) for a 40 years period = **160 non independent simulations**

These examples having 600 and 160 tests for a single experiment are impossible to run in an efficient way without using a workflow management solution.

How to run EC-Earth using Autosubmit

With **Autosubmit** any user can run EC-Earth experiments, from the most simpler cases to the more complex ones. Inside the **runtime/autosubmit** folder there are available all the files needed to do that:

copyruntime.sh : upload sources to remote cluster, call ecconf

compilation.sh : compile all the required model components

eceesm.sh or ece-nemo.sh : run the simulation

| LOCAL SETUP |
| REMOTE SETUP |
| Chunk 1 |
| ... |
| Chunk N |

automatically managed by AUTOSUBMIT

Continuous integration & robustness

Auto-EC-Earth provides a set of templates and auxiliary libraries extending the ones available in the EC-Earth runtime by adding a more robust **deployment**, **initial conditions** set up, **outclasses** handling, automated **post-processing** and data **archiving**. Applying **continuous integration** by using a **testing suite** provides **robustness** to the project. Additionally, weekly tests are performed automatically using the workflow manager. Using this approach, **a representative set of cases are checked and evaluated every week**.

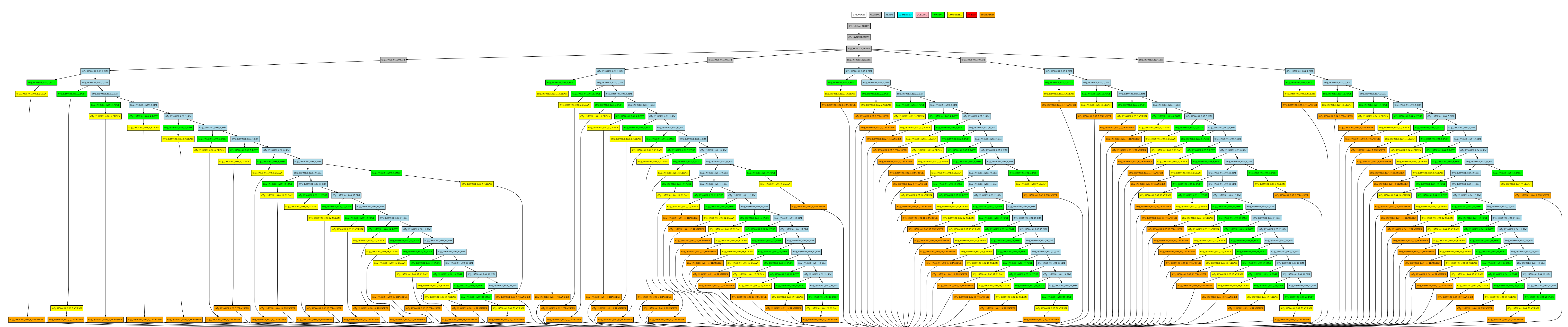| MARENOSTRUM 4 | T255L91-ORCA1L75 cold start |
	T255L91-ORCA1L75 restart
	T255L91 cold start
	T255L91-ORCA1L75-LIM3-LPJG cold start
	ORCA1L75-LIM3 cold start
	ORCA1L75-LIM3 restart
	T511L91-ORCA025L75 cold start
	T511L91-ORCA025L75 restart
CCA	ORCA1L75-LIM3
	T255L91-ORCA1L75-LIM3 restart
	T255L91-ORCA1L75-LIM3 cold start
NORD3	T255L91-ORCA1L75-LIM3 restart

Reproducibility

Fig. 1: reproducibilty experiment t06y

The reproducibility test allows to compare experiments against observational data or two similar experiments between them, taking into account the chaotic nature of Earth System Models. It is useful to **evaluate the impact from changing platforms, computational optimizations, compilers or library versions**. The acceptance / reproducibility test consists in different steps:

1. Run two ensembles of several members and years of simulation, depending on the configuration to analyze. The standard is 5 members and 20 years.

2. Running EC-mean to get the climatology and the Reichler & Kim (R&K) performance indices of each run. This results can be used to compare one experiment to observational data. In this case, CMIP5 database results are used.

3. Cast the R&K indices into a format suitable to compare two similar experiments.

4. A statistical comparison is done using a Kolmogorov test between two experiments, analyzing if significant differences are found between both.

The R&K performance indices can provide us information about how well the configuration is simulating our climate, the Kolmogorov test and R&K indices comparison between two similar experiments with one technical change (different compilation flags for example) can tell us if the technical change done is safe or not.

Autosubmit features

On top to manage complexity and failure, facilitate robust development cycles and reproducible experiments, Autosubmit provides many more features:

- Easily **copy** experiments and configurations (e.g. from the testing suite)
- **Visualize** and share the workflow status at any time
- **Wrap** different and concurrent tasks or sequential jobs in vertical and horizontal packages to execute them on a single job maximizing the utilization of the resources

- **Migrate** experiments from one user to another
- Generate and visualize **experiment statistics**
- Have all the **log** files (local & remote) together in an accessible location
- Modify the number of start dates / ensemble members or the length of an experiment by changing a parameter

Pablo Echevarria | Miguel Castrillo | Mario Acosta